Implicit Simulation Techniques for Dense Plasma Modeling

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Accurate modeling of dense plasma dynamics is useful for many applications including charged particle driven gas breakdown, vacuum arcs, and laser plasmas. One method for the simulation of dense plasmas using an electromagnetic hybrid kinetic-fluid particle-in-cell (PIC) code LSP [1,2] is discussed. The model makes use of an alternating-direct-implicit (ADI) field solver that includes particle currents using an energy conserving variation of the ADI method. The standard D1 implicit electromagnetic algorithm [3] is modified to include an inertial fluid description for electrons [2]. Additionally, particle collisions and gas breakdown models are included. The field solver is based on an unconditionally Courant stable algorithm [4] developed originally for purely electromagnetic calculations.

The original 3-D ADI PIC algorithm implemented in LSP is similar to the method discussed in Refs. [5,6]. The method relaxes the usual time step constraints on the cyclotron and plasma frequencies. The algorithm eliminates the numerical cooling found in the standard D1 treatment for kinetic particles [7]. Including an inertial fluid electron algorithm provides enhanced energy conservation for highly collisional plasmas.

In the original LSP algorithm, particle momenta are advanced using half the electric field at the old position and time, and half at the new position and time, i.e., using cgs units,

$$\boldsymbol{p}_{n+1/2} = \boldsymbol{p}_{n-1/2} + \Delta t\,\left[\boldsymbol{a}_n + \left(\boldsymbol{p}_{n-1/2} + \boldsymbol{p}_{n+1/2}\right)\times q\boldsymbol{B}_n(\boldsymbol{x}_n)/\left(2\gamma_n mc\right)\right],$$

where Δt is the time increment, n refers to a full time step, $\mathbf{a}_n = [\mathbf{a}_{n-1} + q/m\,\mathbf{E}_{n+1}(\mathbf{x}_{n+1})]/2$ and γ is the relativistic factor. A running sum of the old and new electric fields is stored in $\mathbf{a}_n$. The particle γ at n is obtained by using $\mathbf{a}_{n-1}/2$ to push the energy. The particles are actually pushed twice, the first time $\mathbf{E}_{n+1}(\mathbf{x}_{n+1})$ is set to zero. The fields are then pushed using linear correction terms to predict the effect of $\mathbf{E}_{n+1}(\mathbf{x}_{n+1})$ on the currents. The particles are then pushed adding in the new field contribution.

The new particle velocities from the above equations are obtained from $\boldsymbol{p}_{n+1/2} = \langle\mathbf{T}\rangle\cdot\mathbf{A}$, where $\langle\mathbf{T}\rangle$ is the magnetic field rotation tensor given by,

$$\left\langle\mathbf{T}\right\rangle = \frac{1}{1+\Omega^2}\begin{bmatrix} 1+\Omega_1^2 & \Omega_1\Omega_2+\Omega_3 & \Omega_1\Omega_3-\Omega_2 \\ \Omega_1\Omega_2-\Omega_3 & 1+\Omega_2^2 & \Omega_2\Omega_3+\Omega_1 \\ \Omega_1\Omega_3+\Omega_2 & \Omega_2\Omega_3-\Omega_1 & 1+\Omega_3^2 \end{bmatrix},$$

and $\mathbf{\Omega} = \Delta t\; q\; \mathbf{B_n} / (2\gamma mc)$. Subscripts 1–3 denote the three directions and $\Omega^2 = |\mathbf{\Omega}|^2$. The source vector $\mathbf{A}$ is given by, $\mathbf{A} = \boldsymbol{p}_{n-1/2} + \Delta t\; \boldsymbol{a}_n + \boldsymbol{p}_{n-1/2}\times\mathbf{\Omega}$, and advanced in two steps: $\mathbf{A}_1 = \boldsymbol{p}_{n-1/2} + \mathbf{a}_{n-1}\Delta t/2 + \boldsymbol{p}_{n-1/2}\times\mathbf{\Omega}$, and $\mathbf{A}_2 = \mathbf{E}_{n+1}(\mathbf{x}_{n+1})\Delta t/2$.

The correction terms to the field advance are determined by a perturbation analysis. The new particle velocities are calculated assuming $\mathbf{v} = \mathbf{v}^1 + \delta\mathbf{v}$, where $\mathbf{v}^1$ is the velocity calculated in the first push. For a relativistic analysis, $\delta\gamma = \mathbf{v}\cdot\delta\mathbf{E}$ [$\delta\mathbf{E} = \mathbf{E}_{n+1}(\mathbf{x}_{n+1})$], and we obtain

$$\delta\mathbf{v} = \frac{\Delta t\; q}{\gamma_{n+1/2}m}\left[\left\langle\boldsymbol{T}\right\rangle\cdot\delta\boldsymbol{E} - \mathbf{v}_{n+1/2}\left(\mathbf{v}_{v+1/2}\cdot\delta\boldsymbol{E}\right)\right].$$

We can now construct the perturbed current given by $\delta\mathbf{J} = \rho\delta\mathbf{x}/\delta t$ which has the form $\delta\mathbf{J} = \langle\mathbf{S}\rangle\mathbf{A}\delta\mathbf{E}$, where the susceptibility $\langle\mathbf{S}\rangle$ is given by

$$\langle \boldsymbol{S} \rangle = \frac{\rho \Delta t q}{2\gamma_{n+1/2} m}\left(\langle \boldsymbol{T} \rangle - \mathbf{v}_{n+1/2}\mathbf{v}_{n+1/2}\right).$$

The $\langle \mathbf{S} \rangle$ of each particle is summed after the first push. The LSP algorithm, unlike that of Ref. [6], sums particle currents such that charge is conserved. The current "error," determined by the difference between the predicted ($\delta\mathbf{J}$ does not rigorously conserve charge) and calculated currents in the final particle push, is accumulated and gradually corrected over a specified number of time steps. Additionally, the algorithm is made energy conserving by scattering the individual particle $\langle \mathbf{S} \rangle$ to, and gathering the electric field quantities for the momentum push from, the same staggered half-grid positions as the current.

New terms associated with $\langle \mathbf{S} \rangle$ are included in the electromagnetic field equations,

$$\frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{B} - \boldsymbol{J} - \langle \boldsymbol{S} \rangle \cdot \boldsymbol{E} \quad \text{and} \quad \frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E},$$

where $\boldsymbol{J}$ is the kinetic and fluid particle current densities. Although not discussed here, regions can be specified with arbitrary electric permittivity and magnetic permeability. The full tensor expression $\langle \mathbf{S} \rangle \cdot \boldsymbol{E}$ is carried in the old implicit LSP solution, however only the diagonal terms can be used in the new solution. So from here on, we ignore off-diagonal terms. We denote time step index with n (n+1/2 indicates the averages of n and n+1 values) and the Cartesian (x, y, z) grid positions are denoted as (i, j, k). Thus, these equations are finite differenced as follows:

$$\frac{E_{x\,i+1/2,j,k}^{\,n+1} - E_{x\,i+1/2,j,k}^{\,n}}{\Delta t} = \frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1/2} - B_{z\,i+1/2,j-1/2,k}^{\,n+1/2}}{\Delta y} - \frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1/2} - B_{y\,i+1/2,j,k-1/2}^{\,n+1/2}}{\Delta z}$$

$$-J_{x\,i+1/2,j,k}^{\,n+1/2} - S_{xx}^{n+1} E_{x\,i+1/2,j,k}^{n+1},$$

$$\frac{E_{y\,i,j+1/2,k}^{\,n+1} - E_{y\,i,j+1/2,k}^{\,n}}{\Delta t} = \frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1/2} - B_{x\,i,j+1/2,k-1/2}^{\,n+1/2}}{\Delta z} - \frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1/2} - B_{z\,i-1/2,j+1/2,k}^{\,n+1/2}}{\Delta x}$$

$$-J_{y\,i,j+1/2,k}^{\,n+1/2} - S_{yy}^{n+1} E_{y\,i,j+1/2,k}^{n+1},$$

$$\frac{E_{z\,i,j,k+1/2}^{\,n+1} - E_{z\,i,j,k+1/2}^{\,n}}{\Delta t} = \frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1/2} - B_{y\,i-1/2,j,k+1/2}^{\,n+1/2}}{\Delta x} - \frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1/2} - B_{x\,i,j+1/2,k-1/2}^{\,n+1/2}}{\Delta z}$$

$$-J_{z\,i,j,k+1/2}^{\,n+1/2} - S_{zz}^{n+1} E_{z\,i,j,k+1/2}^{n+1},$$

$$\frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1} - B_{x\,i,j+1/2,k+1/2}^{\,n}}{\Delta t} = \frac{E_{y\,i,j+1/2,k+1}^{\,n+1/2} - E_{y\,i,j+1/2,k}^{\,n+1/2}}{\Delta z} - \frac{E_{z\,i,j+1,k+1/2}^{\,n+1/2} - E_{z\,i,j,k+1/2}^{\,n+1/2}}{\Delta y},$$

$$\frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1} - B_{y\,i+1/2,j,k+1/2}^{\,n}}{\Delta t} = \frac{E_{z\,i+1,j,k+1/2}^{\,n+1/2} - E_{z\,i,j,k+1/2}^{\,n+1/2}}{\Delta x} - \frac{E_{x\,i+1/2,j,k+1}^{\,n+1/2} - E_{x\,i+1/2,j,k}^{\,n+1/2}}{\Delta z},$$

$$\frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1} - B_{z\,i+1/2,j+1/2,k}^{\,n}}{\Delta t} = \frac{E_{x\,i+1/2,j+1,k}^{\,n+1/2} - E_{x\,i+1/2,j,k}^{\,n+1/2}}{\Delta y} - \frac{E_{y\,i+1,j+1/2,k}^{\,n+1/2} - E_{y\,i,j+1/2,k}^{\,n+1/2}}{\Delta x}.$$

In the standard implicit field solver of LSP, the above equation is solved iteratively using the ADI method. This involves sweeping through the three coordinate directions. In each sweep in a given direction, the fields are cast such that they are implicit in that direction and explicit in the other two. Each sweep requires the inversion of a tridiagonal matrix. After each iteration, convergence to a specified tolerance is tested, typically 10^{-5}.

Following the method developed in Ref. [4] for purely electromagnetic calculations, we now break up the above equation into two ½Δt pushes. The inclusion of particle currents is straightforward, accomplished by including ½ contributions in each step. The susceptibility terms, however, contain only n+1 electric field values. We have found empirically that by treating these terms as the current and correcting in the second half push, the new set of equations are made stable as well. Thus, in the first ½ step with intermediate time values denoted by n+1/2, the new set of equations are given by,

$$\frac{E_{x\,i+1/2,j,k}^{\,n+1/2}-E_{x\,i+1/2,j,k}^{\,n}}{\Delta t/2}=\frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1/2}-B_{z\,i+1/2,j-1/2,k}^{\,n+1/2}}{\Delta y}-\frac{B_{y\,i+1/2,j,k+1/2}^{\,n}-B_{y\,i+1/2,j,k-1/2}^{\,n}}{\Delta z}$$

$$-J_{x\,i+1/2,j,k}^{\,n+1/2}-S_{xx}^{n+1}E_{x\,i+1/2,j,k}^{n+1/2},$$

$$\frac{E_{y\,i,j+1/2,k}^{\,n+1/2}-E_{y\,i,j+1/2,k}^{\,n}}{\Delta t/2}=\frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1/2}-B_{x\,i,j+1/2,k-1/2}^{\,n+1/2}}{\Delta z}-\frac{B_{z\,i+1/2,j+1/2,k}^{\,n}-B_{z\,i-1/2,j+1/2,k}^{\,n}}{\Delta x}$$

$$-J_{y\,i,j+1/2,k}^{\,n+1/2}-S_{yy}^{n+1}E_{y\,i,j+1/2,k}^{n+1/2},$$

$$\frac{E_{z\,i,j,k+1/2}^{\,n+1/2}-E_{z\,i,j,k+1/2}^{\,n}}{\Delta t/2}=\frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1/2}-B_{y\,i-1/2,j,k+1/2}^{\,n+1/2}}{\Delta x}-\frac{B_{x\,i,j+1/2,k+1/2}^{\,n}-B_{x\,i,j+1/2,k-1/2}^{\,n}}{\Delta z}$$

$$-J_{z\,i,j,k+1/2}^{\,n+1/2}-S_{zz}^{n+1}E_{z\,i,j,k+1/2}^{n+1/2},$$

$$\frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1/2}-B_{x\,i,j+1/2,k+1/2}^{\,n}}{\Delta t/2}=\frac{E_{y\,i,j+1/2,k+1}^{\,n+1/2}-E_{y\,i,j+1/2,k}^{\,n+1/2}}{\Delta z}-\frac{E_{z\,i,j+1,k+1/2}^{\,n}-E_{z\,i,j,k+1/2}^{\,n}}{\Delta y}\ ,$$

$$\frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1/2}-B_{y\,i+1/2,j,k+1/2}^{\,n}}{\Delta t/2}=\frac{E_{z\,i+1,j,k+1/2}^{\,n+1/2}-E_{z\,i,j,k+1/2}^{\,n+1/2}}{\Delta x}-\frac{E_{x\,i+1/2,j,k+1}^{\,n}-E_{x\,i+1/2,j,k}^{\,n}}{\Delta z}\ ,$$

$$\frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1/2}-B_{z\,i+1/2,j+1/2,k}^{\,n}}{\Delta t/2}=\frac{E_{x\,i+1/2,j+1,k}^{\,n+1/2}-E_{x\,i+1/2,j,k}^{\,n+1/2}}{\Delta y}-\frac{E_{y\,i+1,j+1/2,k}^{\,n}-E_{y\,i,j+1/2,k}^{\,n}}{\Delta x}\ ,$$

In the second push, we solve for the full time step fields using old and intermediate field values while correcting the susceptibility terms,

$$\frac{E_{x\,i+1/2,j,k}^{\,n+1}-E_{x\,i+1/2,j,k}^{\,n+1/2}}{\Delta t/2}=\frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1/2}-B_{z\,i+1/2,j-1/2,k}^{\,n+1/2}}{\Delta y}-\frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1}-B_{y\,i+1/2,j,k-1/2}^{\,n+1}}{\Delta z}$$

$$-J_{x\,i+1/2,j,k}^{\,n+1/2}-S_{xx}^{n+1}\left[2E_{x\,i+1/2,j,k}^{n+1}-E_{x\,i+1/2,j,k}^{n+1/2}\right],$$

$$\frac{E_{y\,i,j+1/2,k}^{\,n+1}-E_{y\,i,j+1/2,k}^{\,n+1/2}}{\Delta t/2}=\frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1/2}-B_{x\,i,j+1/2,k-1/2}^{\,n+1/2}}{\Delta z}-\frac{B_{z\,i+1/2,j+1/2,k}^{\,n+1}-B_{z\,i-1/2,j+1/2,k}^{\,n+1}}{\Delta x}$$

$$-J_{y\,i,j+1/2,k}^{\,n+1/2}-S_{yy}^{n+1}\left[2E_{y\,i,j+1/2,k}^{n+1}-E_{y\,i,j+1/2,k}^{n+1/2}\right],$$

$$\frac{E_{z\,i,j,k+1/2}^{\,n+1}-E_{z\,i,j,k+1/2}^{\,n+1/2}}{\Delta t/2}=\frac{B_{y\,i+1/2,j,k+1/2}^{\,n+1/2}-B_{y\,i-1/2,j,k+1/2}^{\,n+1/2}}{\Delta x}-\frac{B_{x\,i,j+1/2,k+1/2}^{\,n+1}-B_{x\,i,j+1/2,k-1/2}^{\,n+1}}{\Delta z}$$

$$-J_{z\,i,j,k+1/2}^{\,n+1/2}-S_{zz}^{n+1}\left[2E_{z\,i,j,k+1/2}^{n+1}-E_{z\,i,j,k+1/2}^{n+1/2}\right],$$

$$\frac{B_{x\,i,j+1/2,k+1/2}^{\;n+1} - B_{x\,i,j+1/2,k+1/2}^{\;n+1/2}}{\Delta t/2} = \frac{E_{y\,i,j+1/2,k+1}^{\;n+1/2} - E_{y\,i,j+1/2,k}^{\;n+1/2}}{\Delta z} - \frac{E_{z\,i,j+1,k+1/2}^{\;n+1} - E_{z\,i,j,k+1/2}^{\;n+1}}{\Delta y} \,,$$

$$\frac{B_{y\,i+1/2,j,k+1/2}^{\;n+1} - B_{y\,i+1/2,j,k+1/2}^{\;n+1/2}}{\Delta t/2} = \frac{E_{z\,i+1,j,k+1/2}^{\;n+1/2} - E_{z\,i,j,k+1/2}^{\;n+1/2}}{\Delta x} - \frac{E_{x\,i+1/2,j,k+1}^{\;n+1} - E_{x\,i+1/2,j,k}^{\;n+1}}{\Delta z} \,,$$

$$\frac{B_{z\,i+1/2,j+1/2,k}^{\;n+1} - B_{z\,i+1/2,j+1/2,k}^{\;n+1/2}}{\Delta t/2} = \frac{E_{x\,i+1/2,j+1,k}^{\;n+1/2} - E_{x\,i+1/2,j,k}^{\;n+1/2}}{\Delta y} - \frac{E_{y\,i+1,j+1/2,k}^{\;n+1} - E_{y\,i,j+1/2,k}^{\;n+1}}{\Delta x} \,,$$

For the new set of equations in each ½ push, there are three sets of equations that can be solved directly. For example, for each row *i*, in *j*, *k*, the equations combine to yield a tridiagonal matrix that is easily inverted.

The two sets of equations now sum to the original LSP implicit field equations to first order in Δt. This is accomplished without the need of multiple iterations required with the original LSP scheme. These equations are thus solved much faster, particularly in parallel operation where message passing can be time consuming. Individually, however, for each ½ step, the new equations obviously are not centered in the *curl* operators. The impact of this lack of centering is not obvious; we suspect that high-frequency electromagnetic wave phenomena are affected. Typically, these high-frequency waves are intentionally damped anyway since they generally result in non-physical and damaging noise. The old and new algorithms yield nearly identical results in all tests to date.

Two complications arise with the new implicit equations. First, we can no longer make use of the Godfrey time biasing method [8] for damping high-frequency noise. In this method, the curl-*B* operator is biased forwards in time which is no longer possible. An alternate scheme [9] in which the electric field values used in the curl-*E* terms are temporally filtered works quite well. The second complication is the handling of open wave transmitting boundaries. This problem is solved with the substitution of the wave condition for transverse electric fields at the boundary into the magnetic field equation at the ½ grid position from the wave transmitting boundary. This condition must be inserted in the tri-diagonal matrix equation and solved implicitly for stability.

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